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THE FORMULATION OF THE KOHN-HULTHÉN VARIATIONAL PRINCIPLE IN TERMS OF THE SCATTERING OPERATION FORMALISM

by

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Abstract

The Kohn-Hulthén variational principle is expressed in terms of a scattering operator formalism. It is shown that in terms of this formalism the principle can be expressed more abstractly and concisely than heretofore.

1. Introduction

A variational principle has been devised by Hulthén for phase shifts in scattering problems (ref. 1). The principle has been modified and its applications have been extended by Kohn (ref. 2). Both of these authors have set up the variational principle explicitly in terms of scattering phases. However, it is simpler to set up the variational principle in terms of the scattering operator formalism. Furthermore in terms of this formalism the principle is more abstract and more general than in terms of the phase-shift representation. In order to discuss this more abstract formalism, we shall summarize the properties of the scattering operator, using essentially the concepts of Møller (ref. 3), Friedrichs (ref. 4), and Lippman and Schwinger (ref. 5).

2. The Scattering Operator

In scattering problems the Hamiltonian H of the system is broken up into two parts, one of which is called the unperturbed Hamiltonian H_o and the other of which is called the perturbation ϵV. Thus

$$H = H_o + \epsilon V. \tag{1}$$

H_o is so chosen as to have a continuous spectrum.

Let us denote the eigenvalues of H_o by E. Generally the spectrum of H_o is degenerate. We shall therefore introduce accessory dynamical variables which commute with H_o and which together with H_o form a complete set of commuting variables. We shall denote the eigenvalues of these accessory variables collectively by α. We shall then write the eigenfunctions of H_o corresponding to the eigenvalue E and α as $\omega_o(E,\alpha)$, where

$$H_o\omega_o(E,\alpha) = E\omega_o(E,\alpha) \tag{2}$$

$$(\omega_o(E,\alpha),\ \omega_o(E',\alpha')) = \delta(E-E')\delta(\alpha,\alpha'); \tag{3}$$

the left-hand side of (3) means the Hermitian inner product, and $\delta(\alpha,\alpha')$ is a generalized δ-function defined by

$$(4)\qquad \int r(\alpha)\delta(\alpha,\alpha')d\alpha = r(\alpha') \text{ if } \alpha' \text{ is in } \mathcal{J}$$
$$= 0 \text{ otherwise,}$$

where $\mathcal{J}$ is the range of integration. Integration over those variables included in α which lie in the discrete spectrum are to be replaced by summations.

It might be useful to indicate the nature of the variables α in order that they may be thought of in more concrete form. If one considers the scattering of a particle by a perturbing potential, one may take H_0 to be the kinetic energy of the particle and ϵV may be considered as the scattering potential. In this case α might be chosen to be the polar angles which specify the direction of the momentum. One might also consider the scattering of an electron by an atom. H_0 would then be the sum of the kinetic energy operator of the electron and the Hamiltonian of the atom. In this case α would consist of the polar angles which give the direction of the electron's momentum, together with the variables which denote the state of the atom. For an example of a problem of this kind see Moses (ref. 6).

We shall denote an arbitrary state Φ in the H_0 representation by $f(E,\alpha)$ and call it the "representer" in that representation; we write

$$(5)\qquad \Phi \underset{E}{\longleftrightarrow} f(E,\alpha) = (\omega_0(E,\alpha), \Phi)$$

or

$$(5a)\qquad \Phi = \iint f(E,\alpha)\ \omega_0(E,\alpha)d\alpha dE .$$

An operator K in the H_0 representation will be written as K^E; it is defined by

$$(6)\qquad K\Phi \underset{E}{\longleftrightarrow} K^E f(E,\alpha).$$

In particular

$$(7)\qquad H_0^E = E$$

as follows immediately from (2) and (5a). Sometimes it is convenient to write K^E as an integral operator with the kernel or "matrix" $K^E(E,\alpha|E',\alpha')$:

(8) $$K^E f(E,\alpha) = \iint K^E(E,\alpha|E',\alpha')f(E',\alpha')d\alpha' dE'.$$

where

(9) $$K^E(E,\alpha|E',\alpha') = (\omega_o(E,\alpha), K\omega_o(E',\alpha')).$$

For purposes of the scattering operator we are interested in eigenfunctions of H which correspond to eigenvalues lying in the same range and having the same degeneracy as the eigenvalues of H_o. We shall denote the eigenvalues of H by F. To describe such eigenfunctions of H we shall have to introduce operators which commute with H and which, together with H, form a complete set of commuting variables collectively by β. The values of β have the same range as α. It is not generally possible to give β a direct physical meaning, but it is not necessary to do so for our purposes.

The eigenfunctions of H are not unique. We shall be interested in two different sets of eigenfunctions which we shall denote by $\omega^+(F,\beta)$ and $\omega^-(F,\beta)$; these we shall now characterize.

Let us denote the $\omega^{\pm}$ in the H_o representation by $u_{\pm}$:

(10) $$u_{\pm}(E,\alpha|F,\beta) = (\omega_o(E,\alpha), \omega^{\pm}(F,\beta)).$$

The eigenfunctions $\omega^{\pm}$ are characterized by the following equations for $u_{\pm}$:

(11) $$u_{\pm}(E,\alpha|F,\beta) = \delta(E-F)\delta(\alpha,\beta) + \epsilon\gamma_{\pm}(F-E)T_{\pm}(E,\alpha|F,\beta),$$

where $\gamma_{\pm}(\zeta)$ is essentially $\delta_{\mp}(\zeta)$:

(12) $$\gamma_{\pm}(\zeta) = \lim_{\xi \to +0} \frac{1}{\zeta \mp i\xi} = \pm i\pi\delta(\zeta) + P\frac{1}{\zeta}.$$

The letter P in (12) means that in integrations over integrands involving $\frac{1}{\zeta}$ as a factor, the Cauchy principal part is to be used. Also

(13) $$T_{\pm}(E,\alpha|F,\beta) = \iint V^E(E,\alpha|E',\alpha')u_{\pm}(E',\alpha'|F,\beta)d\alpha' dE' = V^E u_{\pm}(E,\alpha|F,\beta),$$

where the operator V^E operates on $u_{\pm}$ insofar as $u_{\pm}$ are functions of E,α.

The scattering operator and its inverse can be obtained in terms of the functions $u_\pm$ as follows: Consider solutions of $\Phi(t)$ of the Schroedinger equation

$$(14) \qquad i\frac{\partial}{\partial t}\Phi(t) = H\Phi(t) \qquad (\hbar = 1).$$

If the limits

$$(15) \qquad \lim_{t \to \pm\infty} e^{iH_0 t}\Phi(t) = \Phi_\pm$$

exist, then the scattering operator S is defined by

$$(16) \qquad \Phi_+ = S\,\Phi_- .$$

If we consider the H_0-representer of $\Phi(t)$:

$$\Phi(t) \underset{E}{\longleftrightarrow} f(E,\alpha;t),$$

we see that two possible solutions to the Schroedinger equation can be written:

$$(17) \qquad f_\pm(E,\alpha;t) = \iint u_\pm(E,\alpha|F,\beta)e^{-iFt}g(F,\beta)\,d\beta\,dF,$$

where $g(F,\beta)$ is a quadratically integrable function which was chosen to correspond to a choice of initial conditions on $f_\pm$ as seen below. Friedrichs (ref. 4) shows that f_- is characterized by

$$(18) \qquad \lim_{t \to -\infty} e^{iEt}f_-(E,\alpha;t) = g(E,\alpha);$$

$$(19) \qquad \lim_{t \to +\infty} e^{iEt}f_-(E,\alpha;t) = \iint S^E(E,\alpha|E',\alpha')g(E'\alpha')\,d\alpha'\,dE',$$

where

$$(20) \qquad S^E(E,\alpha|E',\alpha') = \delta(E-E')\delta(\alpha,\alpha')-2\pi i\epsilon\delta(E-E')T_-(E',\alpha|E',\alpha').$$

We can identify equations (18) and (19) as being equation (15) in the H_0-representation. In particular, if we identify $g(E,\alpha)$ as the H_0-representer of Φ_- and $\iint S^E(E,\alpha|E',\alpha')g(E',\alpha')\,d\alpha'\,dE'$ as the H_0-representer of Φ_+, we see that $S^E(E,\alpha|E',\alpha')$ is just the kernel of the integral operator which gives the

scattering operator S in the H_0-representation.

In a similar way it can be shown that

$$(21) \qquad \lim_{t \to +\infty} e^{iEt} f_+(E,\alpha;t) = g(E,\alpha)$$

$$(22) \qquad \lim_{t \to -\infty} e^{iEt} f_+(E,\alpha;t) = \iint \hat{S}^E(E,\alpha|E',\alpha')g(E',\alpha')d\alpha' dE',$$

where

$$(23) \qquad \hat{S}^E(E,\alpha|E',\alpha') = \delta(E-E')\delta(\alpha,\alpha') + 2\pi i\epsilon\delta(E-E')T_+(E',\alpha|E',\alpha').$$

It is clear that $\hat{S}^E(E,\alpha|E',\alpha')$ is just the kernel of the integral operator which gives the inverse scattering operator S^{-1} in the H_0-representation.

In order to obtain the scattering operator we need only find $T_-(E,\alpha|E,\alpha')$. We shall formulate the variational principle for this function. It should be noted that $T_-(E,\alpha|E,\alpha')$ is the amplitude of the scattered wave in the $\underset{\sim}{x}$-representation. It is easier to work in the H_0-representation because the Green's functions involved are simply γ_--functions; in the $\underset{\sim}{x}$-representation they are considerably more complicated.

3. The Variational Expression

The Kohn-Hulthen variational principle is based upon variations of the following functional $A(\mathcal{T}_\pm)$:

$$(24) \qquad A(\mathcal{T}_\pm) = I(\mathcal{T}_\pm) + \epsilon\mathcal{T}_-(F,\beta'|F,\beta).$$

where

$$(25 \qquad I(\mathcal{T}_\pm) = \lim_{F' \to F} \iint \bar{v}_+(E,\alpha|F',\beta')(H^E-F)v_-(E,\alpha|F,\beta)d\alpha dE$$

$$(26) \qquad v_\pm(E,\alpha|F,\beta) = \delta(E-F)\delta(\alpha,\beta) + \epsilon\gamma_\pm(F-E)\mathcal{T}_\pm(E,\alpha|F,\beta)$$
$$= u_\pm(E,\alpha|F,\beta) + \epsilon\gamma_\pm(F-E)\left[\mathcal{T}_\pm(E,\alpha|F,\beta) - T_\pm(E,\alpha|F,\beta)\right].$$

The bar means the complex conjugate.

The functions $\mathcal{T}_\pm$ are to be regarded as trial functions for $T_\pm$. We shall prove later that variations of $A(\mathcal{T}_\pm)$ which result from variations of $\mathcal{T}_\pm$ about $T_\pm$ are zero. Hence $A(\mathcal{T}_\pm)$ is an insensitive functional of $\mathcal{T}_\pm$

in the vicinity of $\mathcal{T}_{\pm} = T_{\pm}$ and we can write

(27) $$A(\mathcal{T}_{\pm}) = A(T_{\pm}),$$

where $\mathcal{T}_{\pm}$ approximates $T_{\pm}$. It will also be shown that

(28) $$I(T_{\pm}) = 0$$

and that hence relation (27) can be written

$$\epsilon T_{-}(F,\beta'|F,\beta) \cong I(\mathcal{T}_{\pm})+\epsilon\,\mathcal{T}_{-}(F,\beta'|F,\beta) = A(\mathcal{T}_{\pm})$$

or, equivalently,

(29) $$T_{-}(F,\beta'|F,\beta) \cong \frac{1}{\epsilon}A(\mathcal{T}_{\pm}).$$

Relation (29) is the form of the Kohn-Hulthén principle in terms of the scattering operator formalism. We use trial functions $\mathcal{T}_{\pm}$ in the right-hand side of (29) to obtain a more accurate expression for $T_{-}(F,\beta'|F,\beta)$.

It should be noted that in evaluating the expression (25) for $I(\mathcal{T}_{\pm})$ one must take care not to interchange the limit and the integration processes prematurely. If one takes the limit before carrying out at least part of the integration, the integrand is not defined because one has the product of two symbolic functions $\bar{v}_{+}\, v_{-}$ which have the same arguments in terms of the variables E and F. Products of symbolic functions having the same argument are generally not defined; however if the symbolic functions have different arguments their products can be defined. For example, $(\delta(x))^2$ is not defined, but $\delta(x)\delta(y)$ is.

After some manipulation it is possible to break up the integrand into a sum in which terms involving products of symbolic functions are isolated. The integral over these products can be evaluated and the limit $F' \to F$ is then taken. For the remaining terms it is proper to interchange the integration and limiting processes. The procedure will be illustrated in the proof of the variational procedure and in the discussion of some results.

4. Proof of the Kohn-Hulthén Variational Procedure

We shall first prove equation (28). We have from the definition (25) of $I(\mathcal{T}_\pm)$ and definition (26) for $v_\pm$

$$(30) \qquad I(T_\pm) = \lim_{F' \to F} \iint \bar{u}_+(E,\alpha|F',\beta')(H^E-F)u_-(E,\alpha|F,\beta)d\alpha dE.$$

However, we remember that in the H_0-representation $u_-(E,\alpha|F,\beta)$ is an eigenfunction of H and H^E is the operator H. Hence $H\omega^-(F,\beta) = F\omega^-(F,\beta)$ becomes

$$(31) \qquad H^E u_-(E,\alpha|F,\beta) = Fu_-(E,\alpha|F,\beta)$$

or

$$(32) \qquad (H^E-F)u_-(E,\alpha|F,\beta) = 0.$$

From this it follows that

$$(28) \qquad I(T_\pm) = 0.$$

We shall now show that variations of $A(\mathcal{T}_\pm)$ resulting from independent variations of $\mathcal{T}_\pm$ about $T_\pm$ vanish.

We denote this variation of $A(\mathcal{T}_\pm)$ by $\delta A(\mathcal{T}_\pm)|_{\mathcal{T}_\pm = T_\pm}$; then

$$(33) \qquad \delta A(\mathcal{T}_\pm) = A(T_\pm + \delta T_\pm) - A(T_\pm).$$

Using (24), (25), (26) we have to the first order in $\delta T_\pm$

$$(34) \qquad \begin{aligned} \delta A(\mathcal{T}_\pm) = \lim_{F' \to F} \epsilon \Big[&\iint \bar{u}_+(E,\alpha|F',\beta')(H^E-F)\gamma_-(F-E)\delta T_-(E,\alpha|F,\beta)d\alpha dE \\ &+ \iint \bar{\gamma}_+(F'-E)\delta T_+(E,\alpha|F',\beta')(H^E-F)u_-(E,\sigma|F,\beta)d\alpha dE \Big] \\ &+ \epsilon\ \delta T_-(F,\beta'|F,\beta). \end{aligned}$$

The second term in the right-hand side of equation (34) vanishes because of equation (32).

Let us designate the first integral on the right-hand side of (34) by $A'(T_\pm)$, which we now evaluate.

$$A'(T_{\pm}) = \lim_{F'\to F} \epsilon \iint \bar{u}_{+}(E,\alpha|F',\beta')(H^{E}-F)\gamma_{-}(F-E)\delta T_{-}(E,\alpha|F,\beta)d\alpha dE. \tag{35}$$

Since H is a Hermitian operator and since u_{+} is an eigenfunction of H in the H_0-representation,

$$H^{E}u_{+}(E,\alpha|F',\beta') = F'u_{+}(E,\alpha|F',\beta'); \tag{36}$$

therefore we have

$$\begin{aligned} A'(T_{\pm}) &= \lim_{F'\to F} \epsilon \iint \left[(\bar{H}^{E}-F)\bar{u}_{+}(E,\alpha|F',\beta')\right]\gamma_{-}(F-E)\delta T_{-}(E,\alpha|F,\beta)d\alpha dE \\ &= \lim_{F'\to F} \epsilon \iint \bar{u}_{+}(E,\alpha|F',\beta')(F'-F)\gamma_{-}(F-E)\delta T_{-}(E,\alpha|F,\beta)d\alpha dE. \end{aligned} \tag{37}$$

We note that

$$\begin{aligned} (F'-F)\gamma_{-}(F-E) &= \left[(F'-E)-(F-E)\right]\gamma_{-}(F-E) \\ &= (F'-E)\gamma_{-}(F-E)-(F-E)\gamma_{-}(F-E) \\ &= (F'-E)\gamma_{-}(F-E)-1. \end{aligned} \tag{38}$$

When (38) is used in (37) we have

$$\begin{aligned} A'(T_{\pm}) = \lim_{F'\to F} \epsilon \Big[&\iint \bar{u}_{+}(E,\alpha|F',\beta')(F'-E)\gamma_{-}(F-E)\delta T_{-}(E,\alpha|F,\beta)d\alpha dE \\ &- \iint \bar{u}_{+}(E,\alpha|F',\beta')\delta T_{-}(E,\alpha|F,\beta)d\alpha dE \Big]. \end{aligned} \tag{39}$$

Now from (11) it follows that

$$(F-E)u_{\pm}(E,\alpha|F,\beta) = \epsilon T_{\pm}(E,\alpha|F,\beta). \tag{40}$$

Hence

$$\begin{aligned} A'(T_{\pm}) = \lim_{F'\to F} \epsilon \Big[&\epsilon \iint \bar{T}_{+}(E,\alpha|F',\beta')\gamma_{-}(F-E)\delta T_{-}(E,\alpha|F,\beta)d\alpha dE \\ &- \iint \bar{u}_{+}(E,\alpha|F',\beta')\delta T_{-}(E,\alpha|F,\beta)d\alpha dE \Big]. \end{aligned} \tag{41}$$

Note that in the first of the integrals we no longer have products of symbolic functions, since $T_{\pm}$ and $\delta T_{\mp}$ are well-behaved functions. Only γ_{-} is a symbolic function. In the second integral $\bar{u}_{+}$ is the only symbolic function. Hence we can now interchange the limit and integration processes in both integrals.

It was not possible to do this earlier. Then recognizing that $\gamma_-(\zeta) = \bar{\gamma}_+(\zeta)$, we obtain from (41)

$$A'(T_\pm) = \epsilon\Big[\epsilon \iint \bar{\gamma}_+(F-E)\bar{T}_+(E,\alpha|F,\beta')\delta T_-(E,\alpha|F,\beta)d\alpha dE - \iint \bar{u}_+(E,\alpha|F,\beta')\delta T_-(E,\alpha|F,\beta)d\alpha dE\Big]. \tag{42}$$

Now from (11) it is seen that

$$\epsilon\bar{\gamma}_+(F-E)\bar{T}_+(E,\alpha|F,\beta') = \bar{u}_+(E,\alpha|F,\beta') - \delta(E-F)\delta(\alpha,\beta').$$

Hence

$$\begin{aligned} A'(T_\pm) &= \epsilon\Big[\iint \bar{u}_+(E,\alpha|F,\beta')\delta T_-(E,\alpha|F,\beta)d\alpha dE \\ &\quad - \delta T_-(F,\beta'|F,\beta) - \iint \bar{u}_+(E,\alpha|F,\beta')\delta T_-(E,\alpha|F,\beta)d\alpha dE\Big] \\ &= -\epsilon\, \delta T_-(F,\beta'|F,\beta). \end{aligned} \tag{43}$$

Finally, since

$$\delta A(\mathcal{T}_\pm) = A'(T_\pm) + \epsilon\delta T_-(F,\beta'|F,\beta),$$

we have from (43)

$$\delta A(\mathcal{T}_\pm) = 0 \tag{44}$$

which completes the proof.

5. Explicit form of $A(\mathcal{T}_\pm)$

Although the form of $A(\mathcal{T}_\pm)$ given by equations (24) through (26) is useful for proving the stationary properties of this functional, it is not very convenient for explicit calculation. One can substitute expressions (25) and (26) in (24) and obtain the following:

$$\begin{aligned} A(\mathcal{T}_\pm) &= \epsilon V^E(F,\beta'|F,\beta) \\ &\quad + \epsilon^2\Big\{\iint V^E(F,\beta'|E,\alpha)\gamma_-(F-E)\mathcal{T}_-(E,\alpha|F,\beta)d\alpha dE \\ &\qquad + \iint \bar{\mathcal{T}}_+(E,\alpha|F,\beta')\gamma_-(F-E)V^E(E,\alpha|F,\beta)d\alpha dE \\ &\qquad - \iint \bar{\mathcal{T}}_+(E,\alpha|F,\beta')\gamma_-(F-E)\mathcal{T}_-(E,\alpha|F,\beta)d\alpha dE\Big\} \\ &\quad + \epsilon^3 \iiiint \bar{\mathcal{T}}_+(E,\alpha|F,\beta')\gamma_-(F-E)V^E(E,\alpha|E',\alpha')\gamma_-(F-E')\cdot \\ &\qquad\qquad \mathcal{T}_-(E',\alpha'|F,\beta)d\alpha dE d\alpha' dE'. \end{aligned} \tag{45}$$

The derivation of (45) is straightforward, though one must, as usual, take care in the use of the limit process involved in the definition of $I(\mathcal{T}_{\pm})$.

We shall now indicate a few simple results. First of all we note that $T_{\pm}(E,\alpha|F,\beta)$ can be calculated by a perturbation procedure. Equations (11) through (13) can be combined to form an integral equation for either $u_{\pm}(E,\alpha|F,\beta)$ or $T_{\pm}(E,\alpha|F,\beta)$; this equation can be solved by interation. First one uses the approximation $T_{\pm} \equiv 0$ and inserts this in equation (11) for $u_{\pm}(E,\alpha|F,\beta)$. With this value of $u_{\pm}$, one uses (13) to obtain better approximations for $T_{\pm}$; this procedure can be repeated to obtain any desired degree of accuracy. This method is equivalent to solving for $u_{\pm}$ or for $T_{\pm}$ by using a power series expansion in ϵ. Each iteration used to find $T_{\pm}$ is called a Born approximation for $T_{\pm}$. For example the zeroeth Born approximation for $T_{\pm}(E,\alpha|F,\beta)$ is zero. The first, $V^E(E,\alpha|F,\beta)$, is obtained by using the first Born approximation for $u_{\pm}$, namely $u_{\pm}(E,\alpha|F,\beta)= \delta(E-F)\delta(\alpha,\beta)$, in (13).

Let us use the zeroeth Born approximation for $T_{\pm}$ as a trial function $\mathcal{T}_{\pm}$. That is, let us use as trial functions $\mathcal{T}_{\pm} = 0$. Then we have from (45) and (29)

$$(46) \qquad T_{-}(F,\beta'|F,\beta) \cong V^E(F,\beta'|F,\beta).$$

This is just the first Born approximation to $T_{-}(F,\beta'|F,\beta)$ that would be obtained using the iteration scheme discussed above.

Let us take as trial functions $\mathcal{T}_{\pm}$ the first Born approximation to $T_{\pm}$, namely

$$\mathcal{T}_{\pm}(E,\alpha|F,\beta) = V^E(E,\alpha|F,\beta).$$

Substituting into (45) and using the fact that V is a Hermitian operator, we have

$$T_-(F,\beta'|F,\beta) \cong V^E(F,\beta'|F,\beta)+\epsilon \iint V^E(F,\beta'|E,\alpha)\gamma_-(F-E)\, V^E(E,\alpha|F,\beta)\,d\alpha dE$$
$$+\,\epsilon^2\iiiint V^E(F,\beta'|E,\alpha)\gamma_-(F-E)V^E(E,\alpha|E',\alpha')\gamma_-(F-E')V^E(E',\alpha'|F,\beta)\,d\alpha' dE' d\alpha dE\,. \tag{47}$$

This is just the third Born approximation to $T_-(F,\beta'|F,\beta)$ using the iteration procedure. Kohn* points out that if one uses for $\mathcal{T}_+$ the m-th Born approximation to T_+ and for $\mathcal{T}_-$ the n-th Born approximation to T_-, then the variational expression gives $T_-(F,\beta'|F,\beta)$ accurately to the (m+n+1) approximation. It should be noted, however, that the variational expression in no way can be used as an iterative procedure to obtain T_-, since the Hulthén procedure gives an approximate function to $T_-(E,\alpha|F,\beta)$ only for E = F, whereas one needs trial functions which are defined for general values of E and F for an iterative method.

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* W. Kohn, Private communication.

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